A New Zeolite Structure Determined Using Simulated Annealing and Synchrotron Powder X-ray Diffraction*	X7A

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ERS-7 (EniRicerche-System-7) was first synthesized in 1995 at Eniricerche (now EniTecnologie) in Italy [1], the composition, thermal stability, and adsorption properties all indicating a zeolite compound. High resolution synchrotron X-ray powder diffraction data were collected at X7A from which the unit cell parameters and space group symmetry (Pnma) were determined. Density measurements then indicated that the unit cell contains approximately 48 tetrahedral sites.

The framework structure of ERS-7 was determined by simulated annealing using the approach of Deem and Newsam [2]. Many simulated annealing runs were performed for each possible number of crystallographically unique T-sites, from 6 to 12. From 1000 runs assuming 6 unique and 48 total T-sites per unit cell, 373 unique framework topologies were generated. The correct structure was identified among these by geometry optimizing candidate frameworks, simulating their PXD patterns, and comparing against the experimental pattern. This solution yeilded the best simulated annealing figure-of-merit, an excellent Rietveld refinement, and a reasonable correlation between lattice energy and density. The relatively complicated ERS-7 framework, having 6 unique tetrahedral-sites and 14 unique bridging oxygens can be be constructed in an entirely face-sharing manner from 17-sided picnic-basket shaped cages, such that a one-dimensional 8-membered-ring channel system runs through the handles of the baskets, while the basket bottoms form pockets along the sides of the channels.This work has now been published [3].

Both neutron and synchrotron powder data have also been collected on the deuterated acid form of ERS-7 in order to study the location of catalytically active sites. *Work at UCSB was supported by the MRL Program of the NSF, Award No. DMR96-32716.

[1] Italian Patent Appl. MI94/A 002037 from Eniricerche S.p.A., (1994). [2] M.W. Deem, J.M. Newsam, *Nature*, **342**, 260 (1989). [3] B.J. Campbell, G. Bellussi, L. Carluccio, G. Perego, A.K. Cheetham, D.E. Cox, R. Millini, *Chem. Commun.*, 1725 (1998).

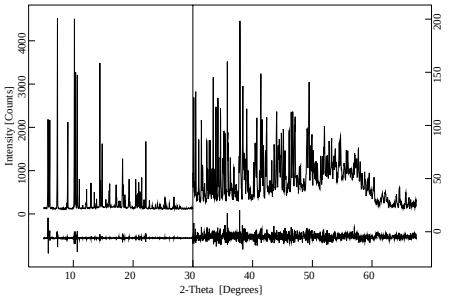

Figure 1. Experimental and difference XRD patterns from the Rietveld refinement of the ERS-7 Structure